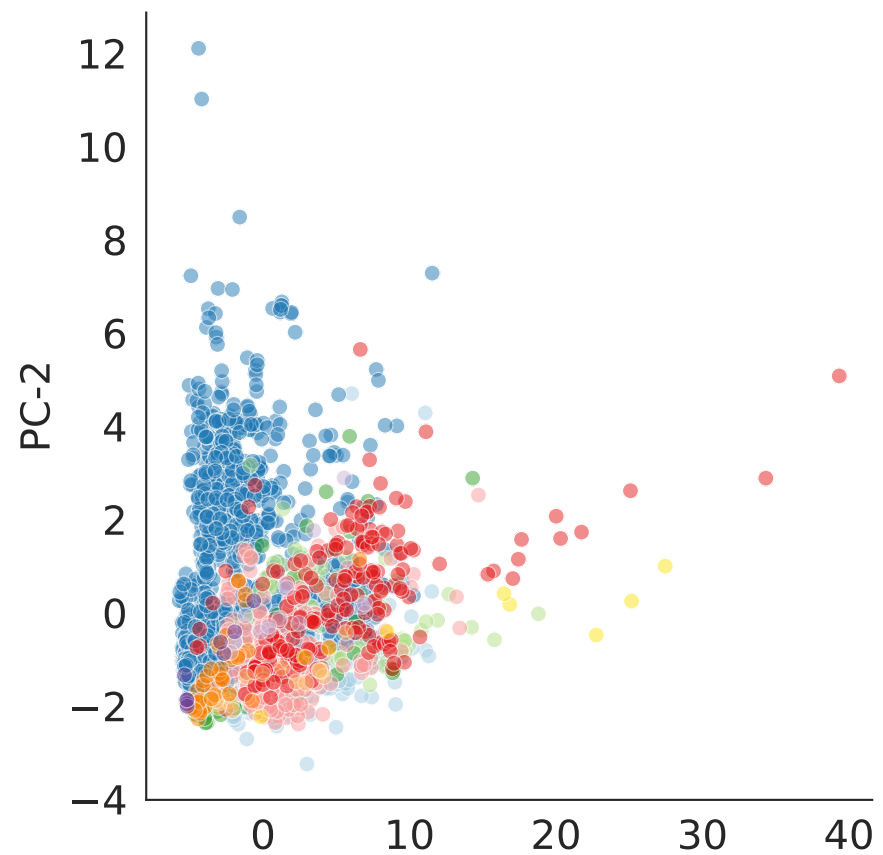
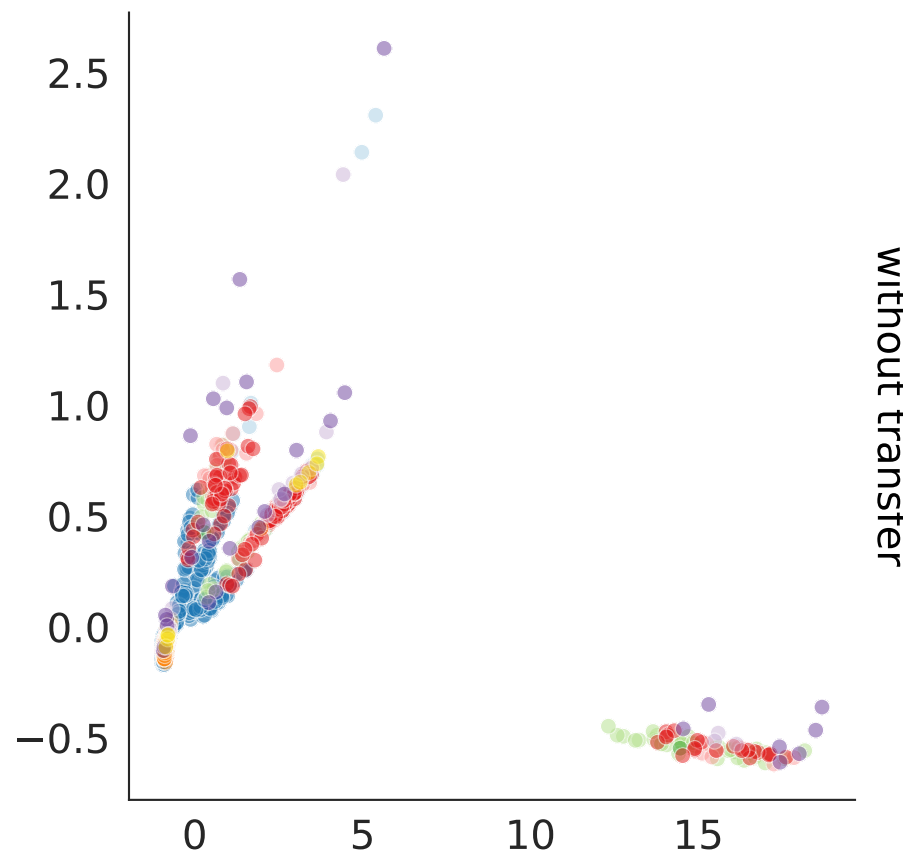


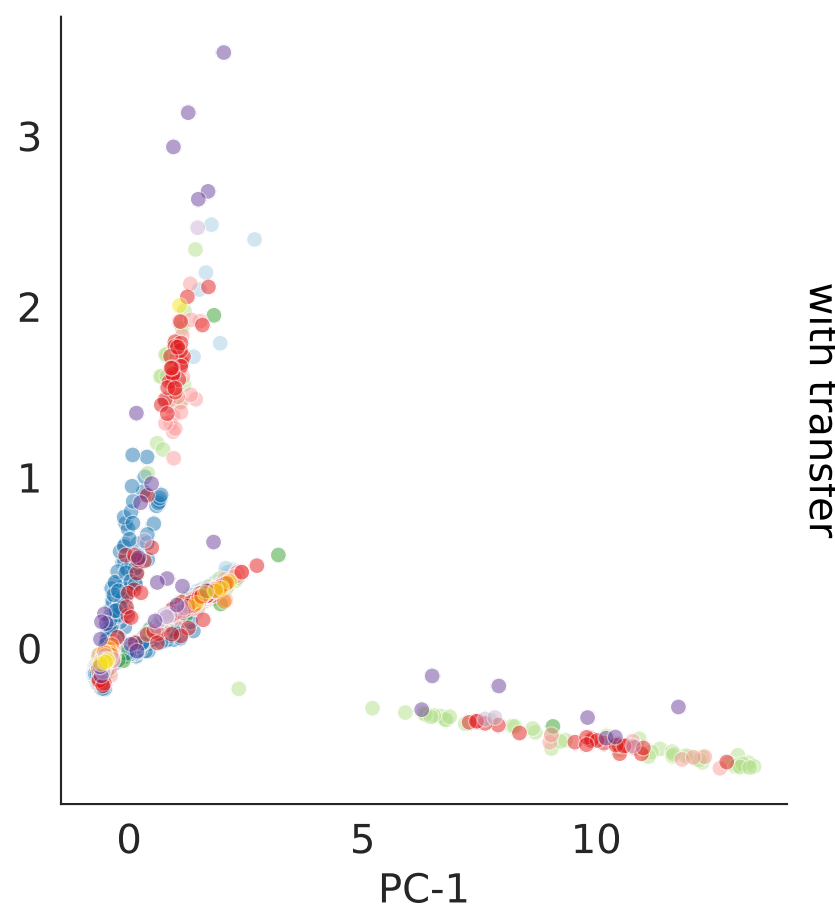
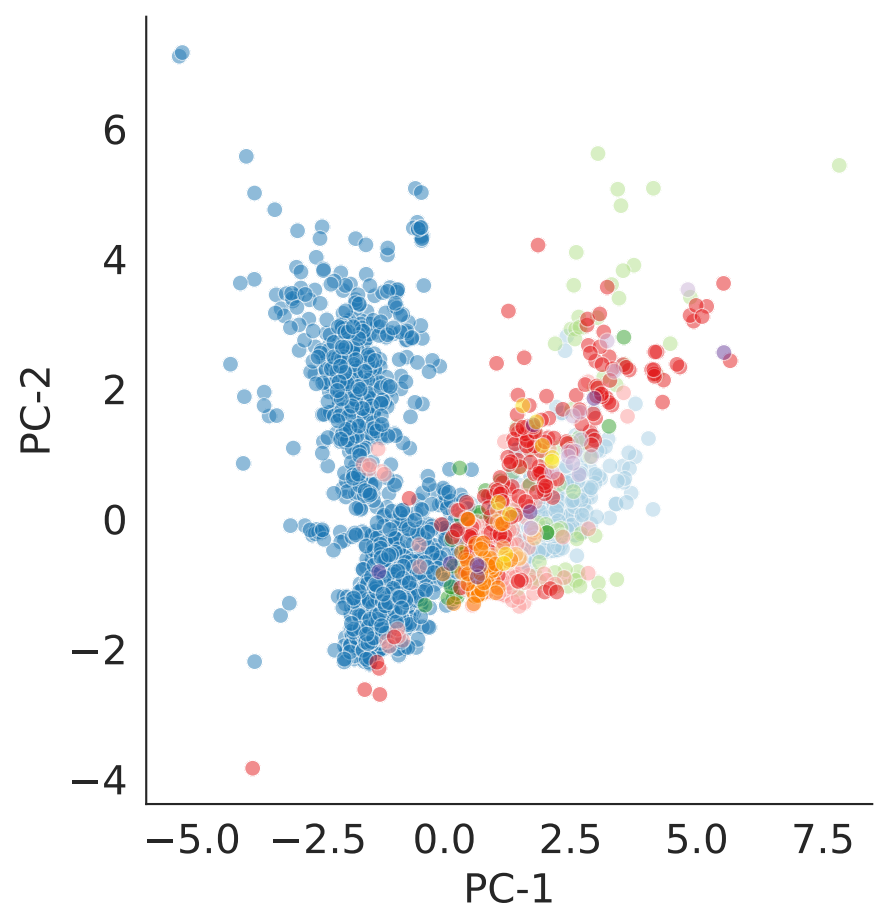
DMPNN



DMPNN with attention



without transfer



with transfer

Acid type

- carboxylic acid
- protonated amine
- C-H acid
- hydroxyl alcohol
- phenol
- amine
- acidic hydroxyl
- thiol
- sulfonic acid
- inorganic
- phosphoric acid